

# Special Topics on Basic EECS I

## VLSI Devices

### Lecture 3

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# Velocity and inverse mass

- Velocity

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} E(\mathbf{k})$$

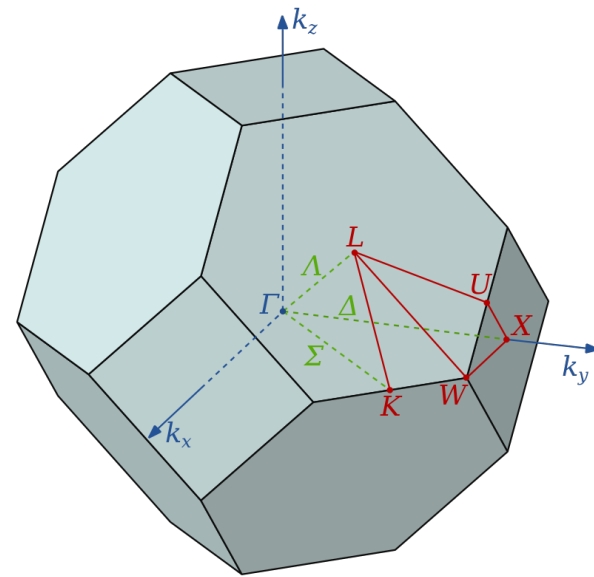
- Inverse mass (its  $ij$  component)

$$m_{ij}^{-1} = \frac{1}{\hbar^2} \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} E(\mathbf{k})$$

- Example) Silicon conduction band

$$E(\mathbf{k}) - E_c = \frac{\hbar^2}{2} \left( \frac{1}{m_{xx}} k_x^2 + \frac{1}{m_{yy}} k_y^2 + \frac{1}{m_{zz}} k_z^2 \right) \quad \sim \text{Taur, Eq. (2.2)}$$

– Among three masses, one is  $m_l$  and the other two are  $m_t$ .



# $\mathbf{v}$ and $m^{-1}$ of an ellipsoidal valley

- Velocity

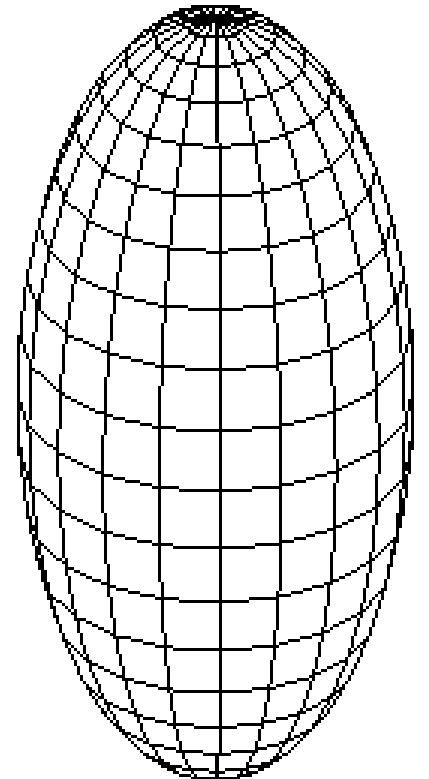
$$\mathbf{v}(\mathbf{k}) = \mathbf{a}_x \frac{\hbar k_x}{m_{xx}} + \mathbf{a}_y \frac{\hbar k_y}{m_{yy}} + \mathbf{a}_z \frac{\hbar k_z}{m_{zz}}$$

- Inverse mass (non-vanishing components)

$$m_{xx}^{-1} = \frac{1}{m_{xx}}, m_{yy}^{-1} = \frac{1}{m_{yy}}, m_{zz}^{-1} = \frac{1}{m_{zz}}$$

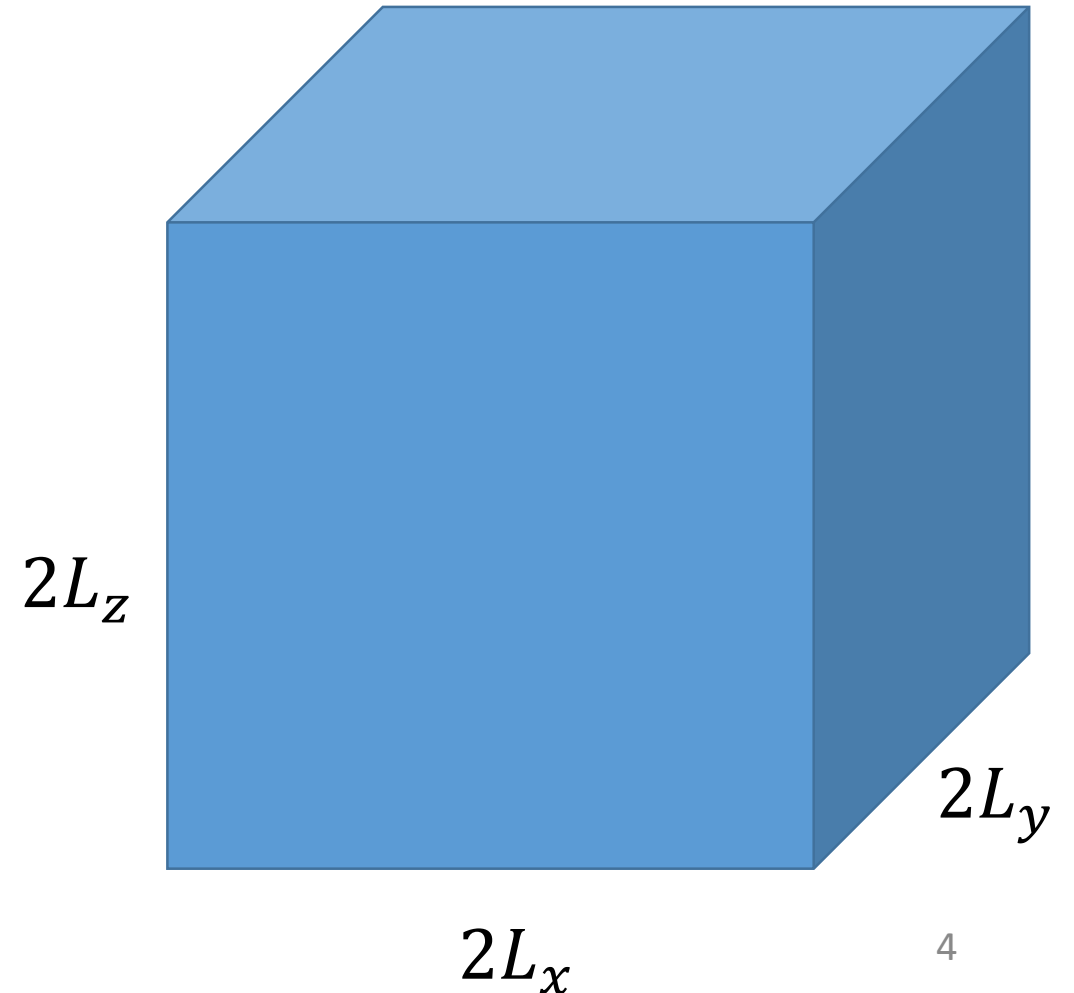
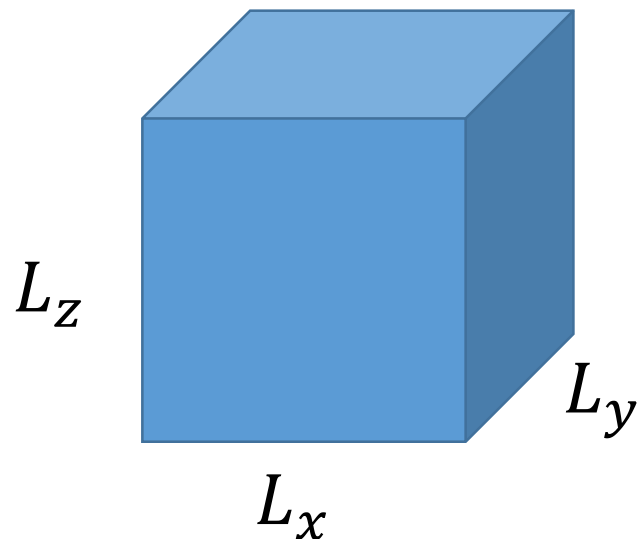
Fast and light  $\rightarrow$

Slow and heavy  $\downarrow$



# Volume of a state in the **k**-space

- A (discrete) **k** point corresponds to an electronic state.
  - One state within  $\frac{(2\pi)^3}{L_x L_y L_z}$  (Left)
  - One state within  $\frac{(2\pi)^3}{8L_x L_y L_z}$  (Right)
  - In general, one state within  $\frac{(2\pi)^3}{Volume}$



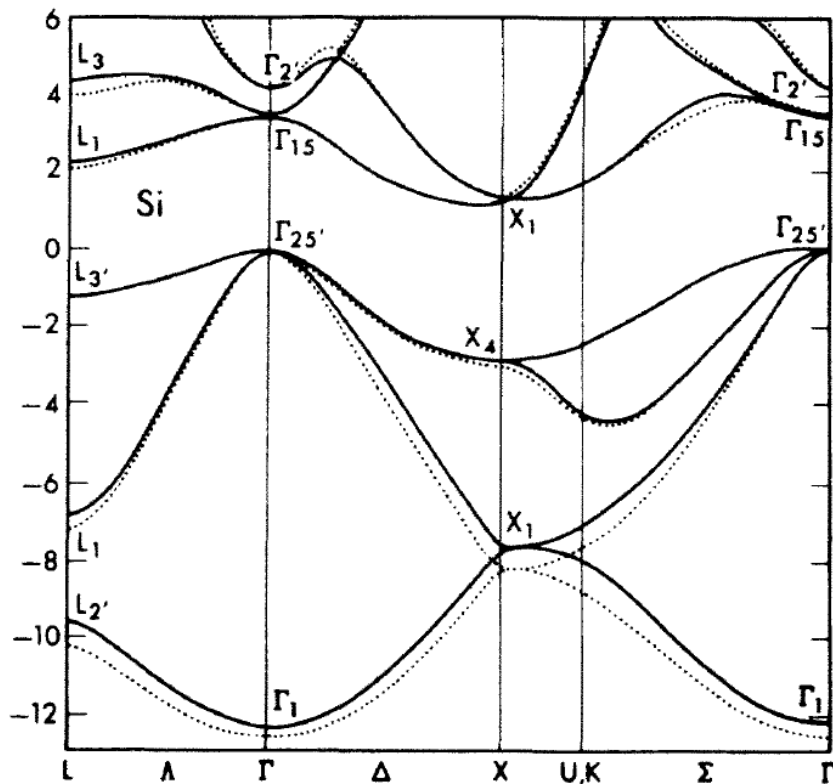
# Number of states inside $dk_x dk_y dk_z$

- Since a state takes  $\frac{(2\pi)^3}{Volume}$ ,
  - Number of states inside  $dk_x dk_y dk_z$  is
$$\frac{Volume}{(2\pi)^3} dk_x dk_y dk_z$$
  - Number of states inside a range of  $[E, E + dE]$ ,
$$\frac{Volume}{(2\pi)^3} \iiint_{E(\mathbf{k}) \in [E, E + dE]} dk_x dk_y dk_z$$

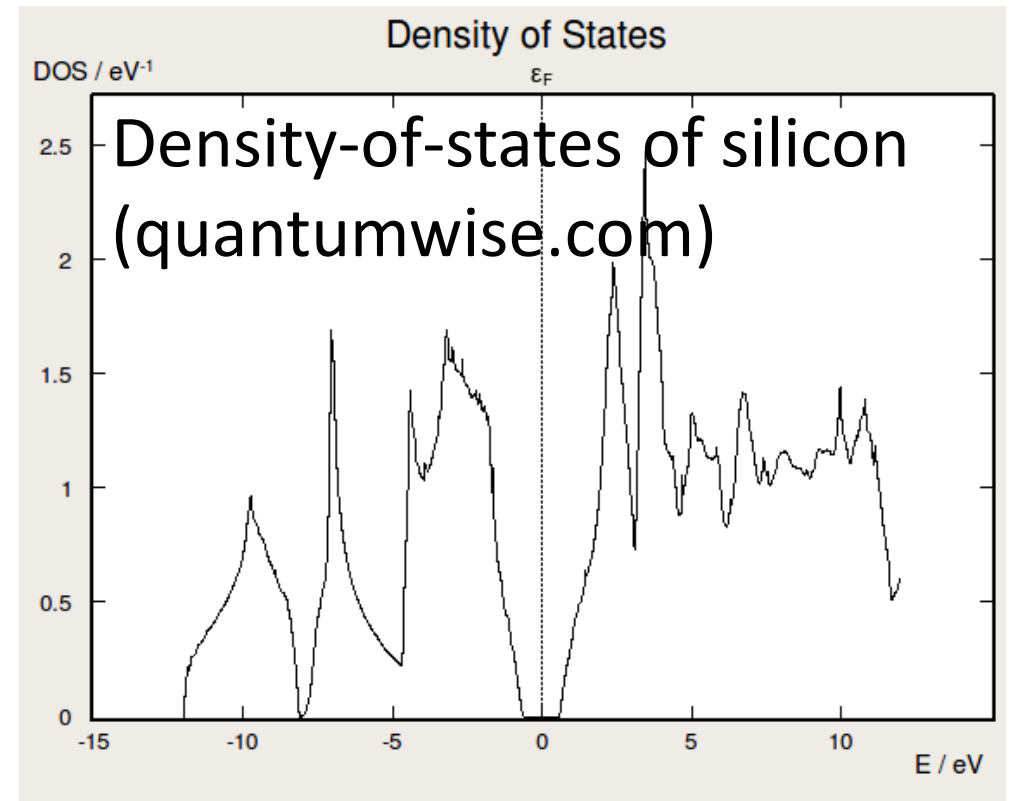
# Density-of-states (DOS)

- DOS,  $N(E)$ , (per spin, per valley)

$$N(E)dE = \frac{1}{(2\pi)^3} \iiint_{E(\mathbf{k}) \in (E, E+dE)} dk_x dk_y dk_z \quad \sim \text{Taur, Eq. (2.1)}$$



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# Density-of-states (DOS) of an ellipsoidal valley

- Volume in the **k**-space

- With  $m^* = (m_{xx}m_{yy}m_{zz})^{\frac{1}{3}}$ ,  
$$\frac{4\pi}{3} \left(\frac{1}{\hbar}\right)^3 (2m^*)^{1.5} (E - E_c)^{1.5}$$

- Therefore, within a range between  $E - E_c$  and  $E - E_c + dE$ ,

$$4\pi \left(\frac{1}{\hbar}\right)^3 (2m_{xx}m_{yy}m_{zz})^{0.5} (E - E_c)^{0.5} dE$$

- DOS of silicon conduction band (per spin, per valley)

$$N(E)dE = \frac{4\pi}{h^3} (2m_l m_t^2)^{0.5} (E - E_c)^{0.5} dE \quad \sim \text{Taur, Eq. (2.3)}$$

# Homework#1

- Non-parabolicity,  $\alpha$

- Consider an isotropic valley,

$$E(1 + \alpha E) = \frac{\hbar^2}{2m^*} k^2$$

- For this valley, express the velocity, the inverse mass, and the DOS using  $E$ .

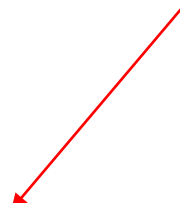


# Electron density

- Number of electrons

$$\# = \sum_{\substack{\text{all } \mathbf{k} \text{ states} \\ \text{occupied}}} 1 = \sum_{\text{all } \mathbf{k} \text{ states}} f(\mathbf{k})$$

0, when empty  
1, when occupied



- Instead of a sum,

$$\# = \sum_{\text{all } \mathbf{k} \text{ states}} f(\mathbf{k}) \approx \frac{\text{Volume}}{(2\pi)^3} \iiint_{\substack{\text{Entire} \\ \mathbf{k} \text{ space}}} f(\mathbf{k}) dk_x dk_y dk_z$$

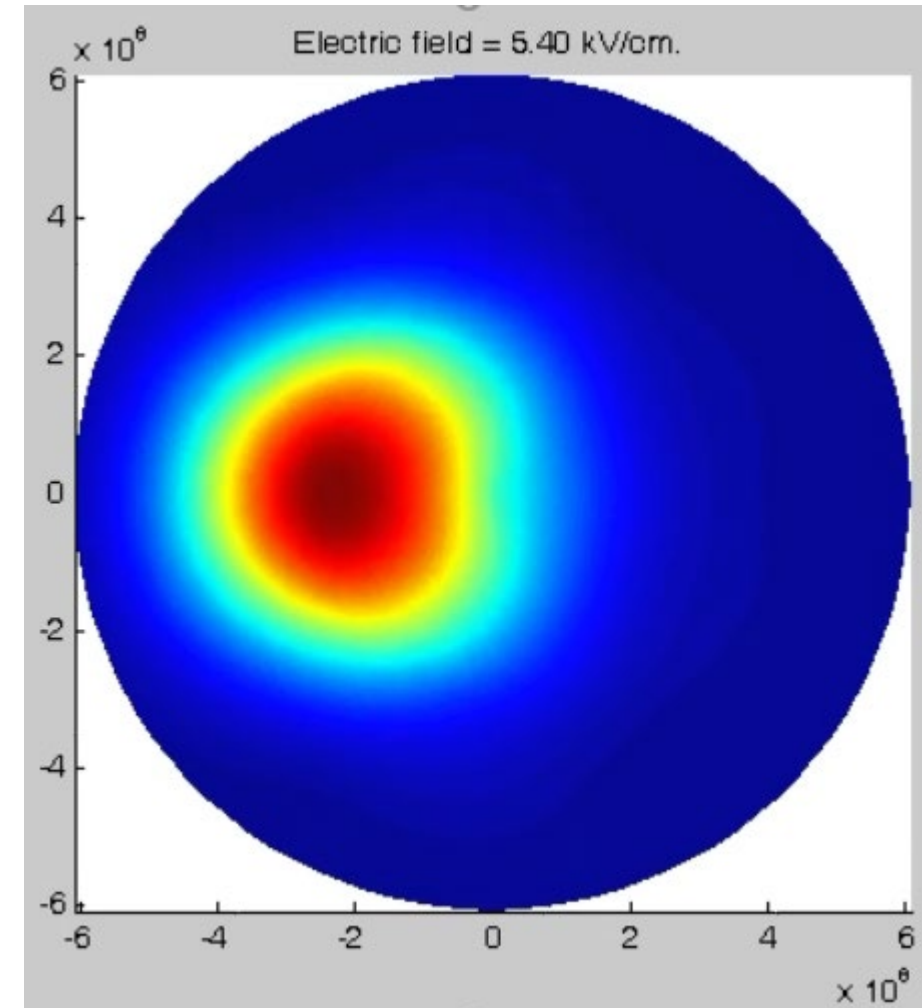
- Electron density (per spin, per valley)

$$n = \frac{\#}{\text{Volume}} = \frac{1}{(2\pi)^3} \iiint_{\substack{\text{Entire} \\ \mathbf{k} \text{ space}}} f(\mathbf{k}) dk_x dk_y dk_z$$

# Distribution function

- $f(\mathbf{k})$  is the distribution function.
  - It is 0, when the state is completely empty.
  - It is 1, when the state is fully occupied.
  - It is in a range of  $[0,1]$ .
  - In general, it is a function of  $\mathbf{k}$ .

Distribution function of  
graphene at a high electric field



# Thank you!